Tunneling through an Aharonov-Bohm ring – effects of dephasing by electron-electron interactions

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(Dated: February 6, 2008)

We develop a non-perturbative numerical method to study a single electron tunneling through an Aharonov-Bohm ring in the presence of bound, interacting electrons. Inelastic processes and spin-flip scattering are properly taken into account. We show that electron-electron interactions described by the Hubbard Hamiltonian lead to strong dephasing and we obtain high transmission probability at $\Phi = \pi$ even at small interaction strength. Depending on the many-electron state on the ring, dephasing can occur in elastic or inelastic channels with or without changing the spin of the scattering electron.

Quantum interference can be studied in mesoscopic systems where the wave nature of electrons plays an important role. Particularly noteworthy are studies of the Aharonov-Bohm (AB) oscillations in mesoscopic rings [1, 2]. Inelastic scattering of electrons is believed to be predominantly responsible for the loss of the phase coherence in such experiments. When an electron interacts with optical phonons, the dephasing only occurs through inelastic processes [3]. At low temperatures the phonon degrees of freedom freeze out, therefore other mechanisms for dephasing, like magnetic impurity scattering or zero-point fluctuations of the electromagnetic environment [4, 5] have been proposed. It is nevertheless believed, that at low temperatures the electron-electron (e-e) interaction is a dominant mechanism for dephasing [6].

The AB geometries have been theoretically studied predominantly by self-consistent mean-field approximations that break down for degenerate levels, which physically happens at very low temperatures [7, 8, 9]. They do not describe transitions in which the symmetry of the wavefunction of bound electrons changes and they are thus inadequate to study decoherence. Renormalisation group techniques have been applied to AB systems [10], where calculations were limited to spinless interacting quantum dot with two levels coupled to reservoirs. Particular attention was devoted to the appearance of Kondo physics induced by changing magnetic flux, however due to limitations to spinless fermions, no spin-flip induced decoherence has been investigated by this method.

To shed some new light on the problem of decoherence, there is obviously a demand for a capable method, that would treat the problem of the scattering of an electron through a limited region where e-e interactions would be exactly taken into account. In this Letter we propose a method that treats e-e interactions by direct diagonalisation using iterative (Lanczos) technique. The method takes into account spin-flip processes, so it can also be used in calculations of spin-polarized transport [11].

We apply the method to study a single-electron transmission through a ring with e-e interactions described by a Hubbard Hamiltonian. We show that dephasing can occur either by a) inelastic processes where the tunneling electron excites bound electrons on the ring or by b) elastic processes, where the tunneling electron changes the symmetry of the degenerate many-electron wavefunction. No exchange of energy is required in the latter case [11, 12, 13, 14]: dephasing occurs because the tunneling electron leaves a trace on its "environment", which consists of bound electrons. In either elastic or inelastic case the dephasing can occur with or without the spin-flip of the scattering electron.

The proposed method is based on the multichannel scattering technique, that was developed for studying the tunneling of a single electron in the presence of scattering by phonons [15, 16]. Since its introduction, it has been successfully applied to a variety of problems where a single electron is coupled to phonon modes [3, 17, 18, 19, 20, 21] and even incorporated into Landauer theory where the influence of electron-phonon scattering on the nonequilibrium electron distribution has been investigated [22]. We now generalise this method to study many-electron problems. While the method can be applied to more general situations, we choose for simplicity a particular physical system which will also serve as a toy-model for the study of the e-e interaction induced dephasing. We thus consider an AB ring coupled to two ideal one-dimensional leads, see Fig. (1). The ring is described by a Hubbard-type Hamiltonian

$$H_{\rm ring} = \sum_{j,\sigma} \left(\epsilon\, c_{j,\sigma}{}^\dagger c_{j,\sigma} - t e^{i\phi_j} c_{j+1,\sigma}{}^\dagger c_{j,\sigma} + {\rm h.c.} \right)$$
$$+ U \sum_j c_{j,\uparrow}{}^\dagger c_{j,\uparrow} c_{j,\downarrow}{}^\dagger c_{j,\downarrow} \tag{1}$$

The operator $c_{j,\sigma}{}^\dagger$ creates an electron with spin σ at site j and we make a formal identification $c_{7,\sigma}{}^\dagger = c_{1,\sigma}{}^\dagger$. The phases ϕ_j describe phase changes due to magnetic flux penetrating the ring. The leads are described by the
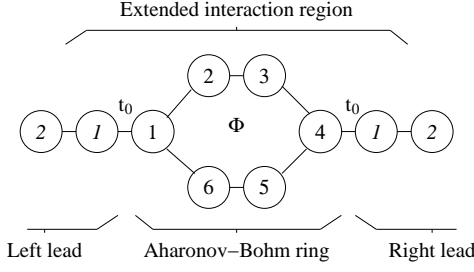
FIG. 1: Aharonov-Bohm ring. Magnetic flux Φ penetrates the center of the ring.

tight-binding Hamiltonian

$$H_{\text{lead}} = -t_{\text{lead}} \sum_{i,\sigma} a_{i+1,\sigma}^{\dagger} a_{i,\sigma} + \text{h.c.}$$
$$-t_{\text{lead}} \sum_{i,\sigma} b_{i+1,\sigma}^{\dagger} b_{i,\sigma} + \text{h.c.}$$

The operator $a_{i,\sigma}^{\dagger}$ creates an electron with spin σ at site i on the left lead, while the operator $b_{i,\sigma}^{\dagger}$ does the same on the right lead. The ring is coupled to the electrodes with coupling constants t_0:

$$H_c = -t_0 \sum_{\sigma} \left(a_{1,\sigma}^{\dagger} c_{1,\sigma} + \text{h.c.} \right) - t_0 \sum_{\sigma} \left(b_{1,\sigma}^{\dagger} c_{4,\sigma} + \text{h.c.} \right) \tag{2}$$

Our approximation consists of taking into account only those many-electron states in which at most one (scattering) electron is located outside the ring. Before the impact of the electron, there are $n = n_{\uparrow} + n_{\downarrow}$ other electrons bound on the AB ring. We truncate all many-body states, where additional electrons hop from the interacting region to the lead. When physical parameters of the system, $e.g.$ (ϵ, t, U), are chosen in such a way that these n electrons are bound in the interacting region, the approximation is equivalent to neglecting the exponentially decaying tails of the n-electron wavefunction in the leads. Before the scattering, the bound electrons are therefore in one of the n-particle eigenstates of the Hamiltonian H_{ring}, Eq. (1). We denote these states by $|\alpha_i^{\uparrow}\rangle$ and their energies by $\epsilon_i^{\uparrow}$. When an incoming electron with spin up enters the ring, the system is in one of the $n + 1$-particle states which we denote by $|\beta_i\rangle$. These states are not necessarily eigenstates of H_{ring}. After the scattering there is a single electron in one of the leads, while the ring is again in one of the n-particle eigenstates of H_{ring}. This state can either be one of the $|\alpha_i^{\uparrow}\rangle$ states or (if the spin of the scattering electron has been flipped) in one of the n-electron eigenstates with $n_{\uparrow} + 1$ spin-up electrons and $n_{\downarrow} - 1$ spin-down electrons. Spin-flipped states are labeled by $|\alpha_i^{\downarrow}\rangle$ and their energies by $\epsilon_i^{\downarrow}$.

By taking into account only the allowed states, the wave-function that describes the scattering of one elec-

tron on the AB ring is given by

$$|\Psi\rangle = \sum_{i=1}^{\infty} \sum_{j,\sigma} d_{i,j,\sigma}^{\text{L}} a_{i,\sigma}^{\dagger} |\alpha_j^{\sigma}\rangle + \sum_{i=1}^{\infty} \sum_{j,\sigma} d_{i,j,\sigma}^{\text{R}} b_{i,\sigma}^{\dagger} |\alpha_j^{\sigma}\rangle$$
$$+ \sum_j e_j |\beta_j\rangle. \tag{3}$$

We consider a steady-state scattering described by the the Schrödinger equation $H|\Psi\rangle = E|\Psi\rangle$ with $H = H_{\text{ring}} + H_{\text{lead}} + H_c$. We operate on this equation from the left with $\langle\beta_l|$ and using Eq. (3) we obtain

$$-t_0 \sum_{j,\sigma} b_{l,j,\sigma}^{\text{L}} d_{1,j,\sigma}^{\text{L}} - t_0 \sum_{j,\sigma} b_{l,j,\sigma}^{\text{R}} d_{1,j,\sigma}^{\text{R}} + \sum_k h_{l,k} e_k = E e_l, \tag{4}$$

where b's denote scalar products $b_{l,j,\sigma}^{\text{L}} = \langle\beta_l|c_{1,\sigma}^{\dagger}|\alpha_j^{\sigma}\rangle$ and $b_{l,j,\sigma}^{\text{R}} = \langle\beta_l|c_{4,\sigma}^{\dagger}|\alpha_j^{\sigma}\rangle$, while $h_{l,k} = \langle\beta_l|H_{\text{ring}}|\beta_k\rangle$ are the matrix elements of Hamiltonian H_{ring} in the $n + 1$ electron subspace. By operating with $\langle\alpha_j^{\sigma}|a_{1,\sigma}$ from the left we get

$$-t_{\text{lead}} d_{2,j,\sigma}^{\text{L}} - t_0 \sum_k (b_{k,j,\sigma}^{\text{L}})^* e_k + \epsilon_j^{\sigma} d_{1,j,\sigma}^{\text{L}} = E d_{1,j,\sigma}^{\text{L}}. \tag{5}$$

In an open outgoing channel (j,σ) a plane wave can propagate, so that $d_{2,j,\sigma}^{\text{L}} = \exp(ik_{j,\sigma}) d_{1,j,\sigma}^{\text{L}}$. By energy conservation the wave number $k_{j,\sigma}$ is obtained from $\epsilon_0 - 2t_{\text{lead}} \cos(K) = \epsilon_j^{\sigma} - 2t_{\text{lead}} \cos(k_{j,\sigma})$. The energy ϵ_0 is the initial energy of the $n-$ electron bound state on the ring, K is the wave number of the incoming electron, and ϵ_j^{σ} is the final energy of the bound electrons. Eq. (5) can thus be written as

$$d_{1,j,\sigma}^{\text{L}} = \frac{-t_0 \sum_k (b_{k,j,\sigma}^{\text{L}})^* e_k}{(E - \epsilon_j^{\sigma} + t_{\text{lead}} \exp(ik_{j,\sigma}))}. \tag{6}$$

Similar equation can be obtained for exponentially decaying outgoing channels that we also take into account. These are defined through the relation $\epsilon_0 - 2t_{\text{lead}} \cos(K) = \epsilon_j^{\sigma} - 2t_{\text{lead}} \cosh(k_{j,\sigma})$ and $d_{2,j,\sigma}^{\text{L}} = \exp(-\kappa_{j,\sigma}) d_{1,j,\sigma}^{\text{L}}$. Using this and Eq. (6), the leads can be removed (pruned) from the problem [16].

At zero temperature, the electron scatters on the ground state of the $n-$ particle state in the ring, $|\alpha_0^{\uparrow}\rangle$ with the energy ϵ_0. In the incoming channel we have both the incoming and outgoing waves, $d_{m,0,\uparrow}^{\text{L}} = \exp(-iKm) + r \exp(iKm)$. We obtain $d_{2,0,\uparrow}^{\text{L}} = \exp(iK) d_{1,0,\uparrow}^{\text{L}} + \exp(iK) - \exp(-iK)$. The equation for the incoming channel thus contains an additional inhomogeneous term $\exp(iK) - \exp(-iK)$.

Equations (4), (6) and equivalent equations for the outgoing channels in the right lead form a system of equations for unknowns $d_{1,j,\sigma}^{\text{L}}$, $d_{1,j,\sigma}^{\text{R}}$ and e_j. This system is solved for different energies of the incoming electron using the conjugated gradients squared (CGS) method

with a Jacobi preconditioner. The partial transmittivity through channel (j, σ) is given by $T_{j,\sigma}(E) = \sin(k_{j,\sigma})/\sin(K)|d^{\mathrm{R}}_{1,j,\sigma}|^2$. Since the method is based on exact solution of many-electron problem, we can compute transmission at arbitrarily large values of U.

Results can be improved by extending the interaction region, which is solved numerically by the Lanczos method, by adding additional sites from the leads. This procedure increases the computational Hilbert space, and consequently it properly takes into account decaying tails of bound electron wavefunctions in the leads. These improvements mainly lead to energy shifts of the resonance peaks while the general characteristics of the spectra remain unchanged. In principle, the region could be extended until the desired convergence is achieved. In our calculations the interacting region consisted of the ring and one additional site from each lead. In cases where the ground state of the interaction region was degenerate, we averaged the transmittivity spectra over all the degenerate states. The variational space taken into account in our calculation was equivalent to a Hubbard model on 8 sites with no translational symmetry. The system of equations was solved to an accuracy finer than the linewidth in the calculated spectra.

We now investigate the effect of the interactions on an electron as it tunnels through the ring. The on-site energies are $\epsilon = -4.5t_{\mathrm{lead}}$, and the overlap integrals are $t = \sqrt{3}t_{\mathrm{lead}}$, and we set $t_{\mathrm{lead}} = 1$. We have limited the energy of the incident electron to a half of the bandwidth, *e.g.* $E = [-2, 0]$, in order to avoid ionisation of the bound electron on the ring which would lead to two electrons exiting the interaction region. In all cases, the incoming electron was chosen to have spin up.

For a test case we first consider a single electron with spin down bound on the ring. We start with the noninteracting case. In the absence of the magnetic field the transmission reaches unity at the resonance, Fig. (2a). The electron is fully reflected at any incident energy when the magnetic flux is $\Phi = \pi$, Fig. (2b). This is the usual Aharonov-Bohm effect.

We now turn on the interaction. At $\Phi = 0$ we still see a unitary peak at the energy of the single-electron resonance, followed by smaller satellite peaks caused by the interaction, Fig. (2c). At $\Phi = \pi$, when in the absence of U the electron is fully reflected, we obtain very high transmission probability despite relatively small $U = 0.2$, Fig. (2d). In the largest peak the transmission approaches the value $1/2$. Since the incoming electron and the bound electron are not entangled, their total spin is not well defined, therefore the total wavefunction is a superposition of a singlet and a triplet state with equal amplitudes: $|\uparrow\downarrow\rangle = 1/\sqrt{2}(|S = 1, S_z = 0\rangle + |S = 0, S_z = 0\rangle)$. The triplet scattering has zero transmission probability at $\Phi = \pi$ since two electrons with spin-up do not interact. The singlet scattering, however, reaches the unitary

limit at finite U at the main resonance peak. Averaging over both contributions, we get $T = 1/2$.

The spin-flip scattering part of the transmission probability is shown in the inset in Fig. (2d). The spin-flip and normal scattering contribute equally to the total transmission probability. Both are purely elastic with respect to energy changes.

Transmission in the spin-flip channel occurs because a spin-flipped electron loses its phase memory [11]. Transmission without the spin-flip occurs because of the double degeneracy of the ground state of the bound electron. The tunneling electron changes the symmetry of the bound electron wave-function and it thereby acquires a phase shift. Such symmetry-changing transitions are only possible when the electrons interact.

We now focus on the case of several strongly interacting ($U = 1$) bound electrons when the flux is $\Phi = \pi$. When the bound state consists of three electrons with spin up and one electron with spin down ($n_\uparrow = 3, n_\downarrow = 1$, see Fig. (3)) no spin-flip scattering is possible because such processes are energetically impossible. The ground state is however fourfold degenerate and the tunneling electron can get through the ring at finite U by changing the symmetry of the many-electron state on the ring. Since the ground state is degenerate, this process is purely elastic. In the case of $n_\uparrow = 0, n_\downarrow = 4$ the ground state is non-degenerate, however the spin-flip processes are energetically allowed. We therefore obtain transmission probability only in spin-flipped channels. Since in this case the ground state is not degenerate, the transmission consists of purely inelastic processes.

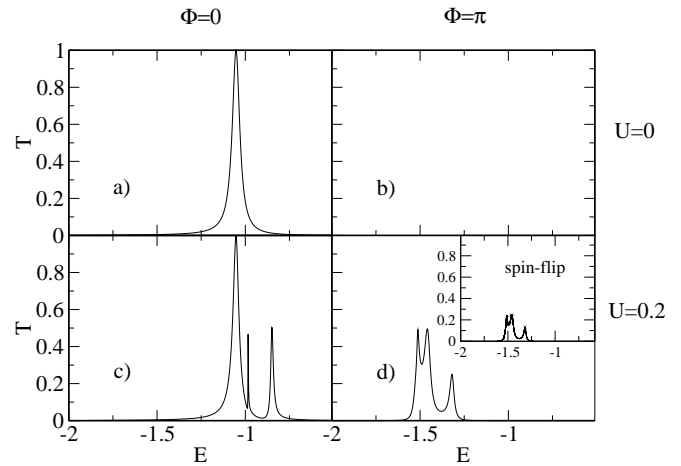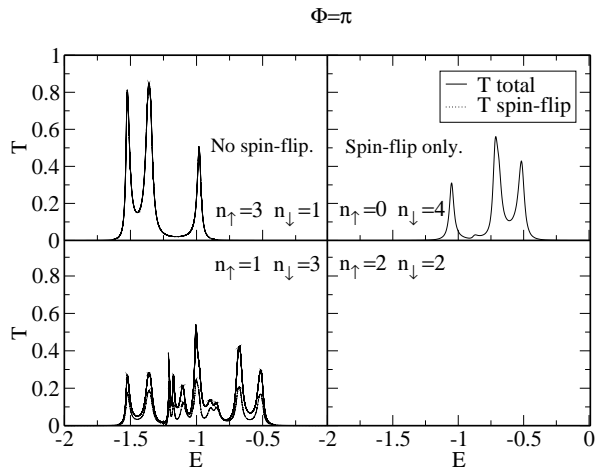In the case when the ground state is degenerate and

FIG. 2: Transmission probability as a function of the incident electron energy for one electron with spin down bound on the ring. The incoming electron had the spin up. The coupling to the lead is $t_0 = 0.4$. In all cases transmission is purely elastic.

FIG. 3: Transmission probability as a function of the incident electron energy for $n_\uparrow$ $(n_\downarrow)$ electrons with spin up (down). Incoming electron had spin up. Interaction $U = 1.0$, coupling constant $t_0 = 0.3$.
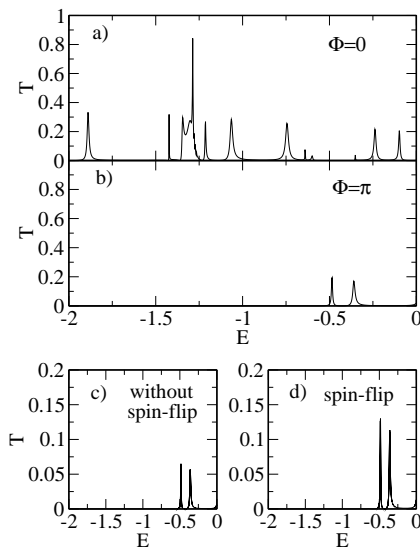

FIG. 4: Transmission probability as a function of incident electron energy. for $n_\uparrow = 2, n_\downarrow = 2$, $U = 15$ and $\epsilon = -20$.

the spin-flips are allowed, we expect dephasing to occur with or without spin flip. Such is the case of $n_\uparrow = 1, n_\downarrow = 3$. The transmittivity without spin-flip is purely elastic, while the spin-flip processes are predominantly elastic, with small contribution from inelastic channels. Finally, for $n_\uparrow = 2, n_\downarrow = 2$ electrons are fully reflected from the ring since there are no allowed spin-flip nor symmetry-changed channels.

Finally we show the influence of large $U = 15$ on the

case of $n_\uparrow = 2, n_\downarrow = 2$, where at $U = 1$ due to widely spaced many-electron levels transmission remained zero in the whole interval of incoming electron energy. At large $U = 15$ the energy difference between the nondegenerate ground state and the first excited state decreases in comparison with $U = 1$ case, as the states become compressed in the lower Hubbard band. We changed the on-site energy to $\epsilon = -20$ in order to keep the electrons bound on the ring. At $\Phi = 0$ there are several energies at which the electron can resonantly tunnel through the ring, Fig. (4a). At $\Phi = \pi$, the electron can only tunnel inelastically. The energy difference to the first excited state in the n electron Hubbard band is approximately 1.4. We find indeed that only the electrons that are more than 1.4 above the bottom of the energy band can tunnel, Fig. (4b). Such inelastic processes occur both without (Fig. 4c) or with spin-flip (Fig. 4d).

Using a simple model and a new numerical method we have extracted the essential physics of tunneling through the AB ring. In particular we have focused on the the role of e-e interactions on dephasing. While the proposed method clearly has some limitations (small interacting regions, inability to describe ionization processes, neglect of many-body effects in the leads), it nevertheless gives precise answers to the question: 'What are the main dephasing mechanisms caused by the e-e interaction?'

A particle can tunnel through AB ring at $\Phi = \pi$ elastically by a) changing the symmetry of the many-electron state which is possible in the case of degeneracy or b) by flipping the spin. Tunneling can also occur in the inelastic channel by exciting the many-electron state on the ring into an excited state with or without the spin-flip. Depending on the number of bound electrons, their total spin, degeneracy of the ground state and available energy of the incoming electron, the total transmission can be composed of partial transmissions caused by either one of the listed processes.

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